LA-UR-21-22836
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Title: Final Technical Report for Project #20180474CR: Properties, Theory, and Measurements for Understanding the Function of Heavy Elements

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Intended for: Report

Issued: 2021-03-23

Final Technical Report for Project #20180474CR: Properties, Theory, and Measurements for Understanding the Function of Heavy Elements

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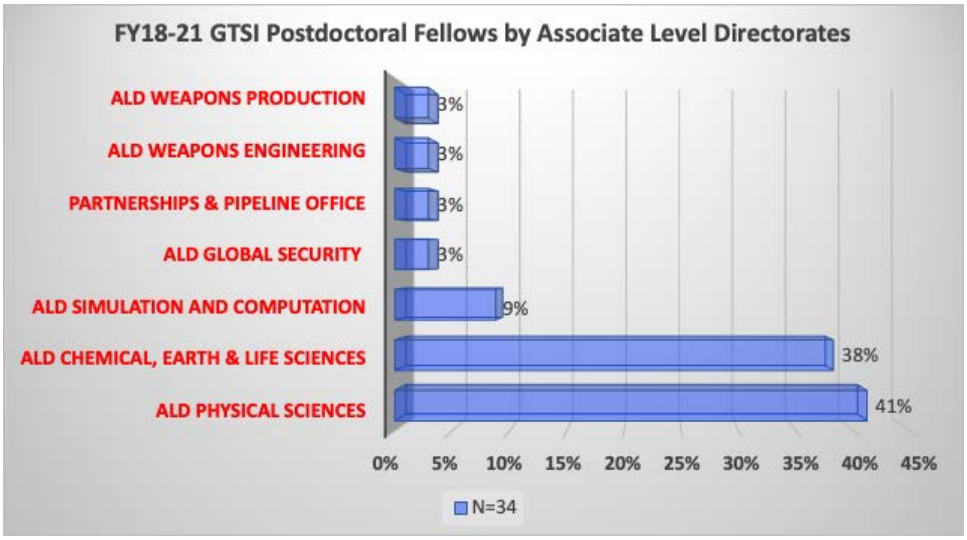
Abstract

The FY18-20 Laboratory Directed Research and Development (LDRD) funded *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* aim has been to advance heavy element science in a comprehensive project connecting targeted research with Los Alamos mission imperatives. The mechanisms for project implementation were (1) support of a multi-year broad-based postdoctoral fellows project, (2) a summer student fellows research project and two seminar series, and (3) organization of structured workshops and integrated educational and career development opportunities. The project was successfully administered by the Glenn T. Seaborg Institute (GTSI) for Transactinium Science and has shown to be an exceptional investment in supporting the Los Alamos National Laboratory (LANL) mission areas requiring heavy element and actinide science by attracting and funding the future generation of scientists and engineers. This project exhibited its value across the laboratory in heavy element and actinide science areas include materials, material properties, signatures, modeling, predictions, fabrication, detection, disposal, global security implications, forensics, and the specialized science surrounding plutonium, uranium, and their surrogates as fuels for energy and nuclear weapons. In this report, the GTSI project staff documents the "high return on investment" implementation as measured against the successes of previous actinide research and science-based projects and as evidenced by the retention of 30% of G.T. Seaborg Postdoctoral Fellows as permanent employees. With additional funding through LDRD Reserve funding during this project period, the GTSI expanded its support for heavy element and actinide science research with a Visiting Research Seaborg Scholar and a Rapid Response Small Projects call. These innovations have served to advance GTSI pursuits as communicated in our FY21-23 LDRD Proposal *Project#: 20210527CR Seaborg Institute: Center for Advancing Actinide Science and Technology at LANL.*

Background and Research Objectives

Founded at LANL in 1997, the GTSI mission has been to: (1) maintain and enhance U.S. capabilities in actinide science and technology; (2) attract and retain the workforce of actinide scientists and engineers needed to meet the needs of our nation; (3) educate and train Laboratory staff, technicians, students, visiting scientists, and faculty at all educational levels in actinide science; and (4) provide expert advice and forums to address LANL and national issues concerning defense and energy applications of the actinides. Central to this mission is the development of sustainable programs that maintain strategic alignment with institutional mission. Of real concern is the recognition that the academic degree programs and research opportunities in nuclear and actinide science are small so that the population of researchers is becoming subcritical at a time when it is crucial for our nation. Strategic focus has been for national laboratories to take a lead role in maintaining core capabilities in nuclear and actinide science by fostering and stewarding early-career scientists' training and research. Heavy element and actinide science and technology, with a particular emphasis on uranium and plutonium, is so important to the present and future scientific health of the laboratory that a sustained institutional commitment is necessary to assure continued excellence. To do this, heavy element and actinide science educational opportunities are needed at many levels.

Historically, LDRD funding for GTSI selected Postdoctoral Fellows working on strategically-selected actinide science projects began in 2004 with an initial $130K investment. **Since its inception in**



2009, the GTSI Postdoctoral Fellows Program has been successful impacting the actinides mission by successfully supporting GTSI Postdoctoral and GRA Fellows and their research as exhibited by a total 668 peer reviewed publications. The GTSI hosts on average 16 Postdoctoral Seaborg Fellows per year in interdisciplinary areas of actinide science. Over the lifespan of the FY18-20 LDRD funded *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project*, the time averaged population of these Seaborg Postdoctoral Fellows represent a broad cross-discipline distribution, to include: 34% in Chemistry; 19% in Materials Physics & Applications; 19% in Materials Science & Technology; 9% in Theory; 7% in Earth and Environmental Sciences; and 9% in Nuclear Engineering and Nonproliferation, Dynamic Experiments and Biology.

The goals of the GTSI Postdoctoral Fellows Program are to advance actinide science, technology, and engineering, relevant to Los Alamos missions, with an emphasis on actinides, and to provide an entry point for exceptionally qualified potential employees. **In the last 10 years, 38 Seaborg Postdoctoral Fellows of 128 or 30% have been converted to LANL staff positions. Engaging selected postdocs and students in multi-year, broad-based research opportunities targeting Los Alamos mission intersects with nuclear energy, nuclear weapons, and global security continues to be a successful Seaborg Institute strategy.** The FY18-20 LDRD Center Research sponsored project entitled *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements* was proposed to support research in heavy element and actinide science relevant to Laboratory mission areas by attracting and funding projects of a future generation of scientists and engineers with a high expectation, based on results from previous actinide research projects, of exceptional science and of retaining them as permanent employees. Nuclear science areas include materials, material properties, science of signatures, modeling, predictions, fabrication, detection, disposal, global security implications, forensics, and the specialized science surrounding actinides and especially plutonium, uranium, and their surrogates as fuels for energy and nuclear weapons. The project goal was to advance nuclear science in a comprehensive project that ties targeted research with Los Alamos mission

Figure 1 Seaborg Postdoctoral Fellows serve as an essential and diverse technical workforce pipeline. Since 2009, there has been a 30% conversion rate to nuclear science engineers, researchers and scientists at LANL and another 13% elsewhere in the DOE Complex.

imperatives. Project implementation was achieved through the support of multi-year broad-based postdoctoral fellows research tasks, and summer student fellows research tasks and education. The project was successfully administered by the Los Alamos GTSI, which is a hub for actinide and transactinide science and engineering research.

Scientific Approach and Results

Knowledge of heavy element and actinide science and engineering continues to be essential to the United States and central to the missions of the DOE and its NNSA laboratories. These areas of expertise include nuclear weapons, global security, energy security, nuclear safeguards, nonproliferation, environmental restoration, and radioactive waste management. With nuclear weapons technology continuing to play an enduring role in defense policy for the foreseeable future, knowledge and expertise in the production, processing, purification, characterization, analysis, and disposal of actinide elements specifically and nuclear materials in general is essential to U.S. national security. Moreover, the risks of global warming, and the environmentally destructive effects of burning coal, nuclear energy is expected to assume a greater role in the nation's electrical energy production in the future. Of the actinide elements, plutonium, uranium and neptunium are especially important to Los Alamos missions. These elements are of technological and scientific interest largely resultant from radioactivity and it is this property, which makes their study particularly challenging. Broadly, there exists a vast range of materials and their understanding important to heavy element and actinide science and engineering. For example, because the lanthanides are in many ways very closely related to the actinides and are important fission products, their study provides important nuclear science information of value to the Los Alamos "all things nuclear" mission, but are less challenging from a security and safety perspective than are actinides.

The basic goal of this project was to support a multi-year, broad-based heavy element and actinide science GTSI Research Fellows tasks or subprojects, organize structured workshops, and implement seminar series to advance actinide science of importance to Los Alamos and the nation. The GTSI Research Fellows LDRD support component of this project leverages GTSI indirect funding along with funds of Science Campaigns and other mission programs. As described elsewhere, the LDRD funds are focused solely on hands-on research, which contribute to peer-reviewed and approved postdoctoral projects. A second goal was to support the Seaborg Institute Actinide Science Summer School, a hands-on laboratory research and educational opportunity that meet the partial requirements of a Ph.D. thesis. This student support component of the project leveraged funding from the LDRD. *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements* Project funded Postdoctoral and Student Fellows have performed research that supports new science at the single-investigator or small-team level in the areas of physics, chemistry, metallurgy, sample production, experimental technique development, measurements, data analysis, theory, and modeling--in short, the entire spectrum of actinides and heavy element-related areas at LANL. **With these insightful strategic goals, a modest $1.32M project enables the scientific endeavors of roughly 12-14 half-time Postdoctoral Fellows and 12-16 GRA Fellows**

Figure 2 Seaborg Postdoctoral Fellows gain hands-on experience working with nuclear materials in unique facilities mentored by leading research staff and world-class subject matter experts.

annually and provides at a minimum of expense for oversight and management of the project. Based on the continuing successes implementing the GTSI mission, we proposed the working hypothesis that Seaborg Research Fellows selected on a competitive basis and whose research was targeted on actinides have demonstrated exceptional return on this strategic investment. We based this expectation on similar success in a previous similarly developed projects based solely on actinides science.

The research and educational programmatic components of the LDRD funded *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements* Project integrate well into the broader actinides science and research mission components implemented by the GTSI. This broader actinides science and research mission is directed at maintaining and enhancing U.S. capabilities in actinide science and technology; educating and training Laboratory staff, technicians, students, visiting scientists, and faculty at all educational levels in actinide science; and providing expert advice and forums to address LANL and national issues concerning defense and energy applications of the actinides. Accordingly, GTSI hosts colloquia, seminars, workshops, and short courses to focus and guide early-career nuclear scientists. Described here are various mechanisms by which the GTSI builds capability and addresses the strategic goals for the Laboratory, outlining those activities supported by non-LDRD funds that aid in providing the environment necessary for the GTSI Postdoctoral Fellows to be successful. Mission components such as actinide topical communication, education and research activities include:

- Technical and Topical Workshops, ex. International Workshop on Theory Frontiers in Actinide Sciences: Chemistry and Materials held 2/2-2/5/20 in Santa Fe, NM;
- Organizational Leadership of the Plutonium Futures Conference,
- Plutonium Science and Research Strategy Implementation,
- Actinide Science Lecture Series,
- Seaborg Institute Seminar Series,
- National Security Education Lecture Series,
- Nuclear and Early Career Lunch Program, and
- Seaborg Visiting Scholars Program.

The *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* research areas include:

- improving our understanding of electronic structure and phonon physics for physical, chemical, mechanical and metallurgical properties of the actinides;
- advancing our knowledge of phase stability and thermodynamics and thermal properties of actinides, actinide alloys and compounds and nuclear materials;
- progressing behavior understanding of the equation of state of actinides, actinide alloys and compounds across pressure, temperature, time, and phase space;
- expanding our understanding of surfaces and interfaces for nuclear materials, structural components for engineered nuclear systems, and containers;
- advancing chemical separations and synthesis processing knowledge and determining their signatures for weapons materials, advanced nuclear energy systems, nuclear forensics, and environmental management;
- expanding our capabilities in detection, measurement, and analysis of signatures of nuclear and radiological materials; and
- improving our knowledge of the environmental behavior and signatures of nuclear materials to ensure proper stewardship.

Accordingly, the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* was designed to capture science that goes beyond strictly actinide science, to include all aspects of heavy element and actinide science. This broad science base has improved our ability to attract and retain the very best early-career scientists so important for the Los Alamos mission in "all things nuclear". Strategic investment has an essential role to promote efforts addressing the outstanding problems being identified and championed by:

- supporting high-risk-high-reward applied science and research to address grand challenges and focus areas within actinide mission space;
- providing short-term seed funding for Postdoctoral Fellows, Graduate Research Student Fellows and their mentors to initiate research aimed at providing the competency and technical underpinnings necessary for multi-year technology development projects;
- fostering sustained excellence and enhanced internal and external visibility in relevant applied science as measured by invited talks, technical reports, peer-reviewed publications, and Postdoctoral Fellows, Graduate Research Student Fellows and their mentors developing research proposals and projects; and
- establishing an intellectual community to facilitate the nucleation of novel ideas to solve timely and important relevant actinide mission scientific and technological problems and initiate rapid deployment of those solutions.

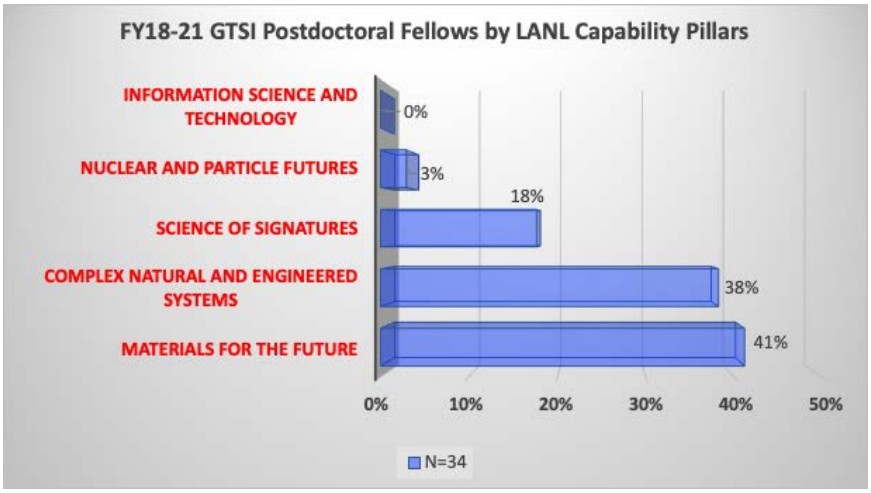
The peer-review process of all *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* funded Research Project Call applications is conducted by cross-institutional Selection Committees. For potential research tasks and nominated candidates, the Seaborg Institute Fellows Selection Committee engaged by the GTSI leadership, selects Seaborg Postdoctoral and Student Research Fellows in a competitive application process. Every effort of the GTSI leadership and the Fellows Selection Committee has been made to ensure that the portfolio of selected proposals spans the strategic breadth of heavy element and actinide science at the laboratory. Calls for applications are publicized electronically and at each lecture of the Seaborg Institute Lecture Series, invited talks given at universities, and at seminars given by the Seaborg Institute leadership. The GTSI leadership and the Fellows Selection Committee actively solicit applications to maintain a balanced portfolio across all the technical areas appropriate to Los Alamos actinide mission space. The successful candidates must be approved for funding by the LANL postdoctoral program and have a clearly defined research proposal that supports new heavy element and actinide science. Calls for applications are made approximately three times a year. Both U.S. and non-U.S. citizens are eligible to apply. Fellow selection is based on the excellence of the science and research in the proposed task, the quality of the candidate, and the strategic value of the proposed research task. Candidates are assessed by the quality of the candidate's transcripts; publication and presentation record; educational background and relevance; and letters of reference. The candidate, working directly with their mentor, craft a research plan that addresses a topic in nuclear science that is broadly connected to the objectives of this project. The Fellows Selection Committee judges the scientific value of the proposed research as well as relevance to the broad goals of heavy element and actinide science at Los Alamos. Successful proposals are clearly defined research proposal that support heavy element and actinide science at the single investigator or small-team level, described in a one-page abstract, and is written by the student and mentor. These research plans address heavy element and actinide science topics connected to the objectives of this project and span the strategic breadth of nuclear science at LANL. Seaborg Postdoctoral Fellows work on a task that connects directly to heavy element and actinide science and that is not otherwise funded. Seaborg Postdoctoral Fellows are funded primarily half-time for the funded research task that connects directly to heavy element and actinide science and that is not otherwise funded. The appointments covered a two-year period, with the

option of a one-year renewal that must be requested in writing for consideration by the G.T. Seaborg Institute leadership and the Internal Advisory Committee.

As a metric of performance, publications of the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* funded Seaborg Fellows have been tracked by the Seaborg Institute leadership. Historically, several of the Seaborg Postdoctoral Fellows' research papers have been featured on the covers of major journals including Nature Chemistry, Nature Materials, and Inorganic Chemistry. **Over the period of this project (FY18-20) in total 122 publications are in print or accepted represents a truly exceptional number considering the difficulties in working with actinides. (See Appendix for a list of all publications by Seaborg Postdoctoral Fellows).** The success of the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* to date has had two peripheral, but important consequences. The first is that some very strong candidates were turned away because of the strict requirement for actinide-only research. The second is that the Los Alamos Science Campaigns have recognized the attraction, recruitment, and retention benefits of previous Seaborg Postdoctoral Fellow subprojects by each contributing approximately $100K/year to fund additional Seaborg Postdoctoral Fellow applicants selected at the same time as the LDRD-funded postdocs, using the same Seaborg application and selection process. Seaborg LDRD Postdoctoral research projects have successfully attracted non-LDRD follow-on funding.

Figure 3 Seaborg Postdoctoral Fellows generated numerous peer-reviewed research paper in high impact publications.

Central to the GTSI mission is the development of sustainable programs that maintain strategic alignment with institutional mission. **The *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* supports approximately supports 41% of funded Seaborg Postdoctoral Fellows focused on research in Materials for the Future Pillar.**



Topics of Seaborg Postdoctoral Fellows in this Pillar included:

- *Measuring the Irradiation Damage Stored Energy in Irradiated Tungsten Materials via Differential Scanning Calorimetry*, Osman El Atwani of MST-8;
- *Small Scale Mechanical Testing of Uranium Materials*, David Frazer of MST-8;
- *High-Precision Plutonium Density Measurements: Immersion Fluid Compatibility, Convective Flow Effects on the Errors of Measuring Self-Heating Samples, and Automating the Process for Glovebox Usage*, Alexandria Marchi of Engineering Institute, NSEC;

- *Gaining New Insight into the Electron Dynamics of Heavy Fermions,* Nicholas Sirica of MPA-CINT;
- *Revealing Hidden Anisotropies in Strongly Correlated Actinide Systems Via Measurements of Thermal Properties Under Strain*, Rico Schoenemann of MPA-MAGLAB;
- *Probing the Origin of the Superconductivity of UTe_2 Using High Magnetic Fields*, You Lai of MPA-MAGLAB;
- *Internal Friction and Elastic Modulus Measurements in Actinides*, Taylor Jacobs of MST-16;
- *Large-scale ab initio Studies of Correlated Electronic Structure of Plutonium Compounds*, Anthony Schlimgen of T-1;
- *Developing A Microstructure Aware Model of Distortion of Alpha-Uranium Components*, Eloisa Zepeda-Alarcon of MST-8;
- *Thermodynamic and dynamic elastic properties of UO_{2+x}*, Jordan Evans of MPA-MAG;
- *High Pressure Properties of Uranium Intermetallic Compounds*, Larissa Huston of M-9;
- *Plutonium Surface Investigations Via Scanning Probe Microscopy Techniques*, Miguel Santiago-Cordoba of MST-7;
- *Quantum Oscillations in Plutonium*, Mark Wartenbe of MST-16; and
- *Development of In-situ Diffraction Analysis and Constitutive Modeling for U-6Nb,* Savage, Daniel of MST-8.

The *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* supports approximately supports 38% of funded Seaborg Postdoctoral Fellows focused on research in Complex Natural and Engineered Systems Pillar. Topics of research in this Pillar included:

- *Theoretical Study of ThO_2 and UO_2 Nanoparticles*, Nestor Aguirre of T-1;
- *Investigation of Surface Chemistry of Uranium Oxide Thin Films at Nanoscale*, Yogesh Sharma of MPA-CINT;
- *Peptoid Polymers as Siderophore Analogues for Actinide Chelation*, David Baumann of B-11;
- *Photochemical Methods for the Synthesis of Organometallic Actinide Complexes*, Justin Pagano of C-IIAC;
- *^{228}Ac as an Imaging and Spectroscopy Agent*, Kelly Aldrich of C-IIAC;
- *Structure, Covalency and Thermodynamic Properties of Actinide (IV)-Organic Complexes*, Sharon Bone of C-IIAC;
- *Synthesis and Chemistry of Actinide Hydrides Using Safe, Mild Conditions,* Karla Erickson of C-IIAC;
- *Ac-225 Targeted alpha-therapy, a new class of antibiotics*, Laura Erickson of C-IIAC;
- *High-Level Theoretical Studies of Actinide-Ligand Bonding Interactions*, Jing Su of T-1;
- *Actinide +3 Aqueous Chemistry*, Zachary Jones of C-IIAC;
- *Advanced in-situ Synchrotron X-ray Scattering Measurements of U/Np/Pu-bearing Compounds at High Pressure-temperature Conditions*, Jason Baker of EES-14;
- *Using Supramolecular Cages to Separate Actinides,* Harrison Root of PT-1; and
- *The Synthesis and Reactivity of Fluorinated Organoactinide Complexes,* S. Cope of C-IIAC.

The *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* supports approximately supports 18% of funded Seaborg Postdoctoral Fellows focused on research in Science of Signatures Pillar. Topics of research in this Pillar included:

- *Improved Photon Data for Advanced Actinide Safeguards Measurements*, Michael Yoho of NEN-1;

- *Developing an HR-ICP-MS Method for Rapid Isotope Measurements of Bulk Nuclear Materials*, Noah Jemison of EES-14;
- *Synthesis and Spectroscopy of Chromogenic Actinide Chelators* Benjamin Stein of C-IIAC; and
- *Understanding the Electronic Structure of Actinide Elements Using EPR Spectroscopy*, Jamie Stull of MST-7.

Within this Pillar, two GTSI Postdoctoral subprojects deserve recognition as high payoff projects. They are the Strategic Interlaboratory Collaboration (LANL-SLAC) entitled

- *Nuclear Provenance of UO_2 Using Multi-modal X-ray Imaging and Spectroscopy Techniques*, Arjen van Veelan of MST-16 and
- *Optical Spectroscopy of Nuclear Materials for Nuclear Safeguards,* Keri Campbell of C-CDE.

Keri campbell's research was successful in developing a technique using LASER Ion Beam spectroscopy (LIBS) to determine phase compositions of uranium oxides and in integrating efforts with T-Division for which the collaboration resulted in significant modification of atomic codes that were designed and employed to model and characterize higher temperature plasmas.

The remainder of **The Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project supports approximately supports 3% of funded Seaborg Postdoctoral Fellows focused on research in Nuclear and Particle Futures Pillar.** Topics of research in this Pillar included:

- *Develop Isotope-Sensitive Method for Absorption Spectroscopy Analysis of Plutonium*, Joshua Bartlett of C-AAC.

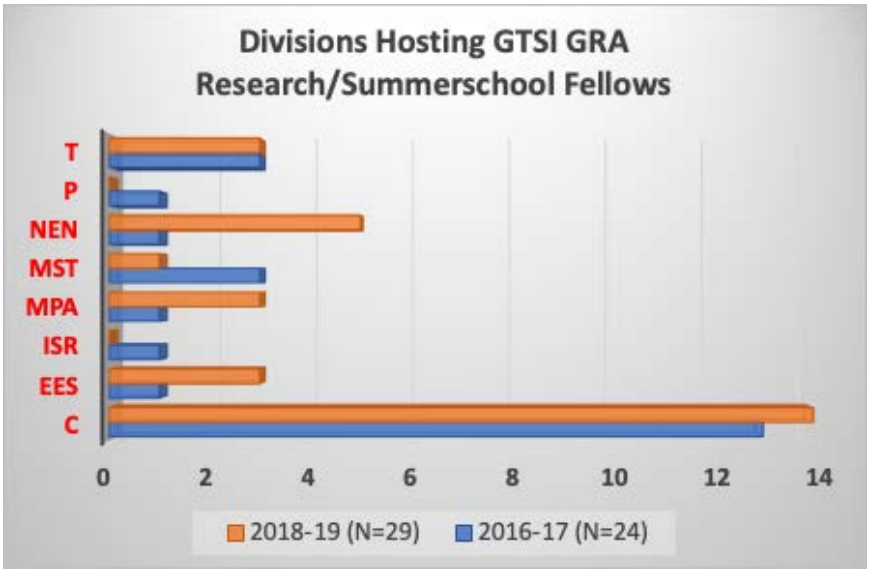
A second strategic component of the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* is Seaborg GRA Research Fellows support component of the project. The **Seaborg Institute Actinide and Materials Science Summer School** - a hands-on laboratory research and educational opportunity, in some cases, meeting the partial requirements of a Ph.D. thesis. Seaborg GRA Fellows support component comes from the GTSI and LDRD. **The LDRD funds were focused solely on hands-on research, which contribute to thesis work.** Through this funding support exists for 10 to 12 outstanding graduate students to participate in the Seaborg Institute Summer Research Fellowships Program. Seaborg GRA Fellowships are funded in broad areas of nuclear and radiochemistry and in actinide science. Fellowships generally run eight to 10 weeks, and give students an opportunity to join Los Alamos scientists in independent research projects that can contribute to their thesis or advanced degree. While at Los Alamos, Research Fellows are encouraged to attend and participate in:

Figure 4 Seaborg Institute Summer School participants attend technical lectures and other professional development events integrated with research opportunities.

- Tours – Los Alamos Windshield Tours, NNSS Test Site Tours, …
- Lecture – Pu Metallurgy, Nuclear Weapons – Past, Present & Future, Nuclear Separations, …
- Professional Development – Grant writing, Presentation Development,…
- Short Course – Radiochemistry, DFT/DMFT, …and

- Peer Networking/Social Engagement – Nuclear Lunches, Early Career Lunches w/ Visiting Scholars,…

Seaborg GRA Fellows are expected to present their research results at a poster session at the end of the summer experience. Seaborg GRA Fellows are generally supported full time over the summer, but in a few cases, students will be supported for a longer time period to conduct thesis work at LANL. **For the period of the FY18-20 *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project,* GTSI funded GRA Fellows published 21 journal publications with the majority of them being first authors. (See Appendix for a list of all publications by Seaborg GRA Research Fellows.)**



Ultimately, the GTSI *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* is designed to promote cutting edge ideas in actinide science, research, and technology with a focus on actinide competency and capability development with international collaboration relevant to all areas of Los Alamos actinide mission space. During this project period, GTSI consistently sought LDRD Reserve funds to facilitate advancement of ideas in outstanding and innovative science and technology and workforce development by enabling the actinide research community at a grassroots level. Examples include the 2019 $100k LRDR Reserve Funding to bring GTSI Visiting Scholar H. Yosuoka to LANL to conduct groundbreaking NMR research on plutonium and other actinide compounds in collaboration with MPA-CMMS postdoctoral researchers and scientists, and the 2020 $200k LRDR Reserve Funding to conduct the first Actinide Small Projects Rapid Response. GTSI seeks to expand those investment opportunities in order to address new actinide challenges. These initiatives have shown to be quite valuable at supporting:

- collaboration with the international actinide research community and providing research seed monies for supporting high-risk-high-reward applied science and research to address grand challenges and focus areas within actinide mission space,
- short-term seed funding for Postdoctoral Fellows, Graduate Research Student Fellows and their mentors to initiate

Figure 5 Seaborg Visiting Scholars provide unparalleled knowledge transfer and scholarship opportunities for Seaborg Postdoctoral Fellows.

research aimed at providing the competency and technical underpinnings necessary for multi-year technology development projects;
- sustained excellence and enhanced internal and external visibility in relevant applied science as measured by invited talks, technical reports, peer-reviewed publications, and Postdoctoral Fellows, Graduate Research Student Fellows and their mentors developing research proposals and projects; and
- intellectual community to facilitate the nucleation of novel ideas to solve timely and important relevant actinide mission scientific and technological problems and initiate rapid deployment of those solutions.

Quantitative metrics of scientific and technical performance cannot be viewed solely by internal advisory and review committees, but should be enhanced by other means, such as, insight of external academic and scientific communities. Leadership within NSEC and the GTSI continuously aim for improvement in the GTSI Research Fellows and other programs. Currently, a challenge is that of concern to GTSI and most basic sciences programs is that of Gender Diversity. Seaborg Fellows Gender Diversity is:

- Seaborg GRA Fellows: 41%/59% Female/Male over 6 yrs. with 50%/50% last 3 yrs. (40%/60% Female/Male national average) and
- Seaborg Postdoctoral Fellows: 32%/68% Female/Male over 6 yrs. with 21%/79% last 3 yrs. (33%/67% Female/Male national average).

With certainty, this is a discipline specific issue and one which we will engage recruiting mentors and hiring research organizations to address. Furthermore, our strategy of improvement is to undergo periodic reviews by a panel of external professional, programmatic and scientific subject matter experts and to act on the recommendations reported by those experts.

Anticipated Impact on Mission

Central to the GTSI vision is the fact that actinide and heavy element science continues to be essential to the U.S. and central to the missions of the DOE and its NNSA laboratories, including nuclear weapons, global security, energy security, nuclear safeguards, nonproliferation, environmental restoration, and radioactive waste management. With nuclear weapons technology continuing to play an enduring role in defense policy for the foreseeable future, knowledge and expertise in the production, processing, purification, characterization, analysis, and disposal of actinide series elements specifically and nuclear materials in general is essential to U.S. national security. Nuclear science and detection technology development is extremely important to nonproliferation and global security. Moreover, the risks of global warming, and the environmentally destructive effects of burning coal are such that energy security growing to include nuclear energy assuming a greater role in the nation's electrical energy production in the future.

Given its charge of fostering the Los Alamos mission competency and capabilities in fundamental actinide and heavy element science, the GTSI continuously seeks to provide opportunity to areas of physics, chemistry, metallurgy, sample production, experimental technique development, measurements, data analysis, theory, and modeling--in short, the entire spectrum of actinides and heavy element-related areas at LANL. The special facilities, instrumentation, and training, existing in only a small number of locations worldwide, are required for safe and secure handling of these elements, distinguishing actinide science from most other research. These capabilities are at the center of our national security mission and the GTSI Leadership will ensure the continued support and strengthening of these assets is a key component of the LANL Lab Agenda Initiative 2.6–Actinide Strategy.

Conclusion

The project, *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* was proposed to support research in nuclear science relevant to Laboratory mission areas by attracting and funding projects of a future generation of scientists and engineers. Successful implementation of the project resulted in the engagement and the support of diverse pool of young bright talented individuals as GTSI Postdoctoral Fellows. The professional development and subsequent research opportunities afforded by this project have shown great value to LANL by (1) improving our understanding of the electronic structure, phase stability, thermodynamics and thermal properties of heavy elements and actinide materials materials and the dynamic behavior of plutonium, uranium, and some of their compounds across pressure, temperature, time, phase space, surfaces and interfaces for nuclear materials; (2) developing advanced chemical separations and synthesis processes, and improving our understanding of the heavy elements and actinide environmental behavior and determine their signatures; and (3) expanding capabilities in detection, measurement, and analysis of signatures of nuclear and radiological materials. Furthermore, the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* has fulfilled its goals as numerous members of its supported early career researcher's population have proven successful candidates as scientists and engineer hires for Los Alamos National Laboratory to continue their work in nuclear science and engineering in support of national mission.

In conclusion the *Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Project* has been shown to:

- Foster sustained excellence and enhanced external visibility in nuclear science at Los Alamos National Laboratory as measured by invited talks, peer-reviewed publications, and Seaborg Institute postdoctoral fellows participation in workshops and conferences.
- Attract and retain a future generation of scientists measured by total project participation and conversions of GRAs to postdocs, and Postdoctoral Fellows to LANL staff.
- Maintain a national resource for the education of present and future scientists and engineers in heavy elements and actinide materials, as measured by Seaborg-sponsored educational functions.
- Establish an intellectual community to facilitate the nucleation of ideas to solve timely and important nuclear technological problems, as measured by participation of Seaborg-sponsored Postdoctoral and GRA Research Fellows and mentors in actinide research workshops and proposals.

Figure 6 GTSI features Seaborg Postdoctoral Fellows research in Special Issues of Actinide Research Quarterly on a biannual basis. These are our most popular ARQ issues.

With additional funding through LDRD Reserve funding during this project period, the GTSI expanded its support for heavy element and actinide science research with a Visiting Research Seaborg Scholar and a Rapid Response Small Projects call. These innovations have served to advance GTSI pursuits as communicated in our FY21-23 LDRD Proposal *Project#: 20210527CR Seaborg Institute: Center for Advancing Actinide Science and Technology at LANL.*

APPENDIX
Project #20180474CR: Properties, Theory, and Measurements for Understanding the Function of Heavy Elements Sponsored Publication

GTSI GRA Research Fellows:

Barker, B. J., et al. (2017). "Photophysical dynamics and relaxation pathways of ligand-to-metal charge-transfer states in the 5f1 [Np(VI)O2Cl4]2– anion." The Journal of Physical Chemistry 121(12): 2353-2360.

Campbell, K. R., et al. (2017). "Phase discrimination of uranium oxides using laser-induced breakdown spectroscopy." Spectrochimica Acta Part B: Atomic Spectroscopy 134(1 August 2017): 91-97.

Coletti, L. M., et al. (2017). "The application of visible absorption spectroscopy to the analysis of uranium in aqueous solutions." Talanta 175: 390-405.

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